

TOROIDAL FULLERENES WITH THE CAYLEY GRAPH STRUCTURE

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ABSTRACT. A central issue in molecular orbital theory is to compute the HOMO-LUMO gap of a molecule, which measures the excitability of the molecule. Thus it would be of interest to learn how to construct a molecule with the prescribed HOMO-LUMO gap. In this paper, we classify all possible structures of fullerene Cayley graphs and compute their spectrum. For any natural number n not divisible by three, we show there exists an infinite family of fullerene graphs with the same HOMO-LUMO gap of size $\frac{2\pi}{\sqrt{3n}} + O(n^{-2})$. Finally, we discuss how to realize those families in three dimensional space.

1. INTRODUCTION

Since the discovery of the first fullerene, Buckminsterfullerene C_{60} , fullerenes have attracted great interest in many scientific disciplines. Many properties of fullerenes can be studied using mathematical tools such as graph theory and group theory. Each fullerene can be represented by a 3-regular graph called the fullerene graph. Its vertices are carbon atoms of the molecule; two vertices are adjacent if there is a bond between corresponding atoms. One special feature of fullerene graphs is that they contain only pentagonal and hexagonal faces.

According to Hückel molecular orbital theory, the energy spectrum of π -electrons of the fullerene can be approximated by eigenvalues of the adjacency matrix of the associated fullerene graph up to a constant multiple [1]. One of the most important information of this energy spectrum is the HOMO-LUMO gap, which is the difference of energies between the highest occupied molecular orbit and the lowest unoccupied molecular orbit. Some partial results about the HOMO-LUMO gaps of certain families of graphs are known [2, 3, 4, 5]. However, it is in general difficult to construct a molecule with the prescribed HOMO-LUMO gap.

In this paper, we will consider a special kind of families of fullerene graphs: those with a Cayley graph structure. A Cayley graph $\mathcal{G}(G, S)$ is a graph that encodes the structure of the group G with a generating set S . It turns out that except for the case of C_{60} which is a Cayley graph on $\text{PSL}_2(\mathbb{F}_5)$ realized on the surface of a sphere, the remaining fullerene Cayley graphs are toroidal provided that they are orientable. There are different techniques to construct a family of toroidal fullerenes, some are based on combinatorial methods [6, 7] and some on geometric approaches [8]. A great advantage of the Cayley graph structure is that all the eigenvalues can be explicitly expressed using representations of the underlying group.

The plan of this paper is as follows. We first classify all possible structures of orientable fullerene Cayley graphs and compute their spectrum. For any natural number n not divisible

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by 3, we show that there exists an infinite family of fullerene graphs with the same HOMO-LUMO gap of size $\frac{2\pi}{\sqrt{3n}} + O(n^{-2})$. Finally we discuss how to realize these families in three dimensional space.

2. CLASSIFICATION OF TOROIDAL FULLERENE

Let G be a group generated by a finite set S . Assume that S is symmetric, namely $S = S^{-1}$. The Cayley graph $X = \mathcal{G}(G, S)$ is defined as follows. Vertices of X are elements in G and two vertices $g_1, g_2 \in G$ are adjacent if $g_1 = g_2 s$ for some $s \in S$. The group G acts on the graph X by left multiplication. Observe that each vertex has exact $|S|$ neighbors and we call X an $|S|$ -regular graph.

$X = \mathcal{G}(G, S)$ is called a fullerene graph if it is 3-regular and it contains only pentagonal and hexagonal faces. In other words, a fullerene graph is a graph endowed with an extra structure: a set of faces enclosed by simple cycles of length five or six, and every edge is exactly shared by two faces. We shall assume that this extra structure is also preserved by the group action. More precisely, if $\gamma = (g, gs_1, \dots, gs_1 \cdots s_n = g)$ is the boundary of a face for some $s_i \in S$, then $g'\gamma$ is the boundary of another face for all elements $g' \in G$. In other word, it is enough to study the faces containing the identity of G and each of this face is represented by a relation $s_1 \cdots s_n = id$.

Let F be a face containing the identity with the boundary $(id, s_1, s_1 \cdots s_n = id)$. If we choose s_1 as the starting vertex, such that the boundary of F is represented by $(s_1, s_1 s_2, \dots, id, s_1)$. If we multiply s_1^{-1} on the left to this boundary, we get $(id, s_2, \dots, s_2 \cdots s_n s_1 = id)$ which represents the boundary of another face containing the identity. Thus, each cyclic permutation of $s_1 \cdots s_n = id$ represents a different face containing the identity. When X is a fullerene graph, which is 3-regular, there are three faces containing the identity and the cyclic permutations of $s_1 \cdots s_n$ can only contain up to three different elements. We conclude that $s_1 \cdots s_n$ must be equal to one of $s_1^5, s_1^6, (s_1 s_2)^3$, and $(s_1 s_2 s_3)^2$.

Write $S = \{a, b, c\}$ and regard G as a quotient of a free group $F_3 = \langle a, b, c \rangle$ by three kinds of relation: the orders of generators, the relations of faces and other relations. We shall first classify the group structures of G without other relations and any finite fullerene graph is isomorphic to a finite quotient of G . We distinguish two cases:

Case (1): all generators have order two, say, $a^2 = b^2 = c^2 = id$.

In this case, a relation of faces must have the form $(ab)^3 = id$, $(abc)^2 = id$, or their conjugations by permutating a, b, c . Note that $(ba)^3 = id$ and $(ab)^3 = id$ represents the same boundary of a face with opposite directions. Consequently, there are two subcases:

Case (1a): three relations of faces are $(abc)^2 = id$, $(bca)^2 = id$ and $(cba)^2 = id$.

Case (1b): three relations of faces are $(ab)^3 = id$, $(bc)^3 = id$ and $(ac)^3 = id$.

Case (2): at least one generator has order not equal to two, say, $a^2 = id, b^2 \neq id, c = b^{-1}$. In this case, a relation of faces must have the form $b^5 = id$, $b^6 = id$, $(ab)^3 = id$ or $(ab^2)^2 = id$. Therefore, there are three subcases:

Case (2a): three relations of faces are $(ab^2)^2 = id$, $(bab)^2 = id$ and $(b^2 a)^2 = id$.

Case (2b): three relations of faces are $b^6 = id$, $(ab)^3 = id$ and $(ba)^3 = id$.

Case (2c): three relations of faces are $b^5 = id$, $(ab)^3 = id$ and $(ba)^3 = id$.

We conclude that

Theorem 1. *A fullerene Cayley graph $\mathcal{G}(G, S)$ is isomorphic to a finite quotient of one of the following five graphs described in terms of generators and relations, and S is the image of S_i under the quotient.*

- $G_1 = \langle a, b, c | a^2 = b^2 = c^2 = (ab)^3 = (ac)^3 = (bc)^3 = id \rangle$;
- $G_2 = \langle a, b, c | a^2 = b^2 = c^2 = (abc)^2 = (bca)^2 = (cab)^2 = id \rangle$;
- $G_3 = \langle a, b | a^2 = (ab^2)^2 = (bab)^2 = (b^2a)^2 = id \rangle$;
- $G_4 = \langle a, b | a^2 = b^6 = (ab)^3 = (ba)^3 = id \rangle$;
- $G_5 = \langle a, b | a^2 = b^5 = (ab)^3 = (ba)^3 = id \rangle$.

It is not hard to prove that G_5 is isomorphic to $\text{PSL}_2(\mathbb{F}_5)$ and in this case the graph is the well-known C_{60} . For the first four cases, X contains only hexagonal faces. Let V , E and F be the number of vertices, edges and faces of X , respectively. The euler characteristic of X is equal to

$$V - E + F = |G| - \frac{3}{2}|G| + \frac{1}{2}|G| = 0.$$

Therefore, X lies on a torus if it is orientable; it lies on a Klein bottle if it is non-orientable. In order to embed X in three dimensional space, we shall assume it is orientable. In the rest of paper, we shall consider finite toroidal fullerene Cayley graphs.

3. GEOMETRIC MODEL OF TOROIDAL FULLERENE CAYLEY GRAPHS

In this section, we will give each G_i a geometric model.

Let Y be the hexagonal tiling of the Euclidean plane \mathbb{R}^2 such that the origin O is the center of a hexagon as shown in Figure 1.

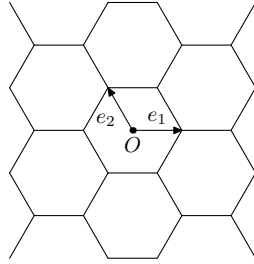


Figure 1: a hexagonal tiling of \mathbb{R}^2

For convenience, we use $\{\vec{e}_1, \vec{e}_2\}$ in Figure 1 as the basis of \mathbb{R}^2 to express linear transformations and translations. The group of affine transformations on \mathbb{R}^2 is the semi-direct product $W = \mathbb{R}^2 \rtimes \text{GL}_2(\mathbb{R})$. More precisely, the action of $(\vec{v}, A) \in W$ on $\vec{u} \in \mathbb{R}^2$ is given by

$$(\vec{v}, A)(\vec{u}) = \vec{v} + A\vec{u},$$

and the group law is

$$(\vec{v}_1, A_1) \cdot (\vec{v}_2, A_2) = (\vec{v}_1 + A_1\vec{v}_2, A_1A_2)$$

The group W contains four different types of elements: rotations, reflections, translations, and glide reflections. Note that only rotations and reflections may have finite orders. We shall construct an explicit embedding σ_i of each group G_i into W and show that it induces a graph isomorphism from $\mathcal{G}(G_i, S_i)$ to Y .

Let $\vec{e}_0 = \vec{e}_1 + \vec{e}_2$ and let $\rho : \text{Aut}(Y) \rightarrow Y$ be the evaluation map given by $\rho(f) = f(\vec{e}_0)$.

Case (a): $G_1 = \langle a, b, c | a^2 = b^2 = c^2 = (abc)^2 = id \rangle$.

Define $\sigma_1 : G_1 \longrightarrow W$ by

$$\begin{aligned}\sigma_1(a) &= \left(\begin{bmatrix} 2 \\ 1 \end{bmatrix}, \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \right), & \sigma_1(b) &= \left(\begin{bmatrix} 3 \\ 3 \end{bmatrix}, \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \right), \\ \sigma_1(c) &= \left(\begin{bmatrix} 1 \\ 2 \end{bmatrix}, \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \right).\end{aligned}$$

Here $\sigma_1(a)$, $\sigma_1(b)$ and $\sigma_1(c)$ are 180° -rotations centered at a_0 , b_0 , c_0 , respectively, as shown in Figure 2.

Case (b): $G_2 = \langle a, b, c | a^2 = b^2 = c^2 = (ab)^3 = (ac)^3 = (bc)^3 = id \rangle$.

Define $\sigma_2 : G_2 \longrightarrow W$ by

$$\begin{aligned}\sigma_2(a) &= \left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 1 & -1 \end{bmatrix} \right), & \sigma_2(b) &= \left(\begin{bmatrix} 3 \\ 3 \end{bmatrix}, \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix} \right), \\ \sigma_2(c) &= \left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} -1 & 1 \\ 0 & 1 \end{bmatrix} \right).\end{aligned}$$

Here $\sigma_2(a)$, $\sigma_2(b)$ and $\sigma_2(c)$ are reflections with respect to the axes a_0 , b_0 , c_0 , respectively as shown in Figure 3.

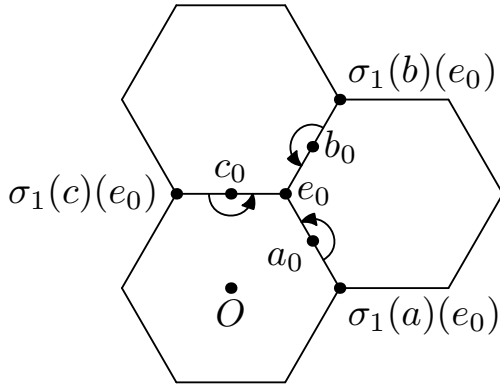


Figure 2: $\rho \circ \sigma_1(G_1)$

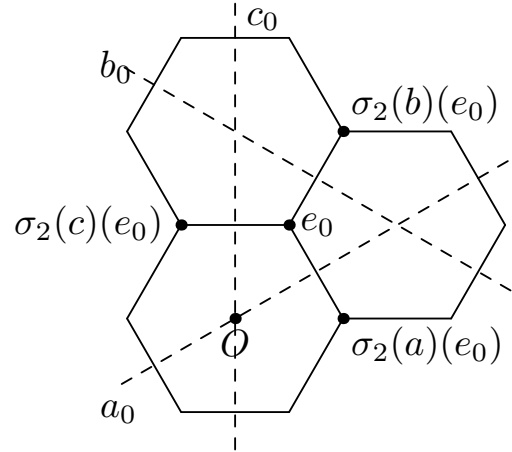


Figure 3: $\rho \circ \sigma_2(G_2)$

Case (c): $G_3 = \langle a, b | a^2 = (ab^2)^2 = (bab)^2 = (b^2a)^2 = id \rangle$.

Define $\sigma_3 : G_3 \longrightarrow W$ by

$$\sigma_3(a) = \left(\begin{bmatrix} 2 \\ 1 \end{bmatrix}, \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \right), \quad \sigma_3(b) = \left(\begin{bmatrix} 1 \\ 2 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 1 & -1 \end{bmatrix} \right).$$

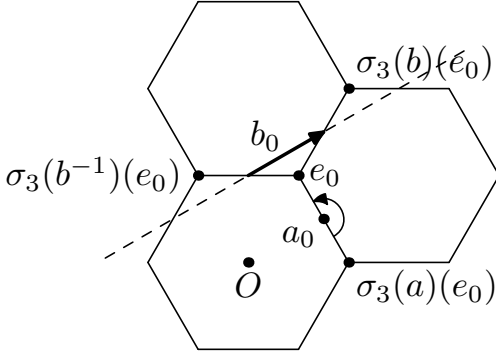
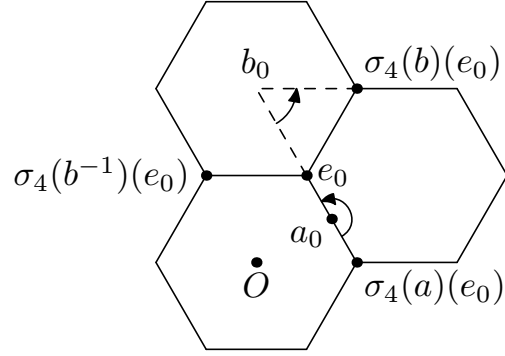
Here $\sigma_3(a)$ is a 180° -rotation around the point a_0 and $\sigma_3(b)$ is a glide reflection with respect to the axis b_0 as shown in Figure 4.

Case (d): $G_4 = \langle a, b | a^2 = b^6 = (ab)^3 = (ba)^3 = id \rangle$.

Define $\sigma_4 : G_4 \longrightarrow W$ by

$$\sigma_4(a) = \left(\begin{bmatrix} 2 \\ 1 \end{bmatrix}, \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \right), \quad \sigma_4(b) = \left(\begin{bmatrix} 2 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 & -1 \\ 1 & 0 \end{bmatrix} \right).$$

Here $\sigma_4(a)$ is a 180° -rotation around the point a_0 and $\sigma_4(b)$ is a 60° -rotation around the point b_0 as shown in Figure 5.

Figure 4: $\rho \circ \sigma_3(G_3)$ Figure 5: $\rho \circ \sigma_4(G_4)$

Observe that ρ induces a graph isomorphism from $\mathcal{G}(\sigma_i(G_i), \sigma_1(S_i))$ to Y for $i = 1, 2, 3, 4$. To show that each σ_i is an isomorphism, we use the following basic propositions in group theory.

Proposition 2. *Let H be a normal subgroup of G and σ be a homomorphism from G to another group G' . If σ from H to $\sigma(H)$ and the induced map of σ from G/H to $\sigma(G)/\sigma(H)$ are both injective, then σ is also injective.*

Proposition 3. *Any surjective homomorphism from \mathbb{Z}^2 to \mathbb{Z}^2 is an isomorphism.*

Let $\vec{v}_1 = 2\vec{e}_1 + \vec{e}_2$, $\vec{v}_2 = \vec{e}_1 + 2\vec{e}_2$ and $T_{\vec{v}}$ denote the translation $\vec{x} \rightarrow \vec{x} + \vec{v}$.

Theorem 4. $\mathcal{G}(G_i, S_i)$ is isomorphic to Y as a graph for $i = 1, 2, 3, 4$.

Proof. Since $\mathcal{G}(\sigma_i(G_i), \sigma_i(S_i))$ is isomorphic to Y as a graph, we only need to show that σ_i is injective and then it induces a graph isomorphism from $\mathcal{G}(G_i, S_i)$ to $\mathcal{G}(\sigma_i(G_i), \sigma_i(S_i))$. We shall find, for each G_i , the translation subgroups H_i and verify that σ_i is injective on both H_i and G_i/H_i and hence σ_i is injective by Proposition 2.

Case (a) Let $H_1 = \langle bc, ba \rangle$. It is easy to check that H_1 is an abelian normal subgroup of G_1 . Since $\sigma_1(H_1) = \langle \sigma_1(bc), \sigma_1(ba) \rangle = \langle T_{\vec{v}_1}, T_{\vec{v}_2} \rangle \cong \mathbb{Z}^2$, we have that H_1 is also isomorphic to \mathbb{Z}^2 . By Proposition 3, σ_1 is injective on H_1 . On the other hand, in G_1/H_1 , $c = b^{-1}$, $a = b^{-1}$ and then $G_1/H_1 = \langle b|b^2 = id \rangle$. Since b is not a translation, we have $\sigma(bH_1) \neq \sigma(H_1)$ and so σ_1 is injective on G_1/H_1 .

Case (b) Let $H_2 = \langle cbca, abac \rangle$. It is easy to check that H_2 is an abelian normal subgroup of G_2 . Since $\sigma_2(H_2) = \langle \sigma_2(abac), \sigma_2(cbca) \rangle = \langle T_{2\vec{v}_1 - \vec{v}_2}, T_{2\vec{v}_2 - \vec{v}_1} \rangle \cong \mathbb{Z}^2$, we have that H_2 is also isomorphic to \mathbb{Z}^2 . By Proposition 3, σ_2 is injective on H_2 . On the other hand, in G_2/H_2 , $c = (aba)^{-1}$ and then $G_2/H_2 = \langle a, b|a^2 = b^2 = (ab)^3 = id \rangle$. Thus $G_2 = \coprod gH_2$, where $g = id, a, b, ab, ba, aba$. Since none of a, b, ab, ba, aba is a translation, σ_2 is injective on G_2/H_2 .

Case (c) Let $H_3 = \langle b^2, baba \rangle$. It is easy to check that H_3 is an abelian normal subgroup of G_3 . Since $\sigma_3(H_3) = \langle \sigma_3(b^2), \sigma_3(baba) \rangle = \langle T_{\vec{v}_1}, T_{2\vec{v}_2 - \vec{v}_1} \rangle \cong \mathbb{Z}^2$, we have that H_3 is also isomorphic to \mathbb{Z}^2 . By Proposition 3, σ_3 is injective on H_3 . On the other hand, $G_3/H_3 = \langle a, b|a^2 = b^2 = (ba)^2 = id \rangle$. Thus $G_3 = \coprod gH_3$, where $g = id, a, b, ab$. Since none of a, b, ab is a translation, σ_3 is injective on G_3/H_3 .

Case (d) Let $H_4 = \langle b^3a, bab^2 \rangle$. It is easy to check that H_4 is an abelian normal subgroup of G_4 . Since $\sigma_4(H_4) = \langle \sigma_4(b^2), \sigma_4(baba) \rangle = \langle T_{2\vec{v}_1 - \vec{v}_2}, T_{2\vec{v}_2 - \vec{v}_1} \rangle \cong \mathbb{Z}^2$, we have that H_4 is also isomorphic to \mathbb{Z}^2 . By Proposition 3, σ_4 is injective on H_4 . On the other hand, in G_4/H_4 , $a = b^{-3}$ and then $G_4/H_4 = \langle b|b^6 = id \rangle$. Thus $G_4 = \coprod b^i H_4$, where $0 \leq i \leq 5$. Since none of b^i is a translation for $1 \leq i \leq 5$, σ_4 is injective on G_4/H_4 . \square

For now on, we identify each G_i with $\sigma_i(G_i)$ as a subgroup of W .

4. FINITE TOROIDAL FULLERENES

The Cayley graphs discussed in the previous section are infinite graphs and they are all isomorphic to the hexagonal tiling Y as graphs. To obtain finite fullerene graphs, we shall consider finite quotients of these graphs. Recall that a torus is obtained as the quotient of the Euclidean plane by a lattice. In our case, the translation subgroup of W plays the same role as lattices. Observe that the translation group T preserving Y is spanned by translations $T_{\vec{v}_1}$ and $T_{\vec{v}_2}$. Thus every finite toroidal fullerene comes from a quotient of $\mathcal{G}(G_i, S_i)$ by a normal subgroup H of G_i contained in T . Observe that $T \subset G_1$ and every subgroup of T is normal in G_1 . Consequently, all finite toroidal fullerenes arise from quotients of $\mathcal{G}(G_1, S_1)$ by its translation subgroups. Let $s = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}$, then we can write the generators a, b and c of G_1 as

$$a = (\vec{v}_1, s), \quad b = (\vec{v}_1 + \vec{v}_2, s), \quad c = (\vec{v}_2, s), \quad \text{and} \quad G_1 = \langle \vec{v}_1, \vec{v}_2 \rangle \rtimes \langle s \rangle \cong \mathbb{Z}^2 \rtimes \mathbb{Z}/2\mathbb{Z}$$

We conclude that

Theorem 5. *Every finite toroidal fullerene is isomorphic to some $X_N = \mathcal{G}(G_N, \{a, b, c\})$, where N is a rank two subgroup of \mathbb{Z}^2 , $G_N = \mathbb{Z}^2/N \rtimes \mathbb{Z}/2\mathbb{Z}$ and $a = (\vec{v}_1, s)$, $b = (\vec{v}_1 + \vec{v}_2, s)$ and $c = (\vec{v}_2, s)$.*

5. SPECTRUM OF A FINITE FULLERENE

In this section, we compute the spectrum of the toroidal fullerene graph X_N . Recall that if Φ is the right regular representation of G_N , then the adjacent matrix of X_N is equal to $\Phi(a) + \Phi(b) + \Phi(c)$. On the other hand, Φ decomposes as the sum of all irreducible representations $\{\Phi_i\}$ of G_N with multiplicity equal to the dimension of Φ_i . Thus, it suffices to compute the eigenvalues of $\Phi_i(a) + \Phi_i(b) + \Phi_i(c)$. Denote by \hat{A} the set of characters of an abelian group A . To find all irreducible representations of G_N , we apply the following theorem [9]:

Theorem 6. *Let $G = A \rtimes H$, where H is a subgroup and A is a normal abelian subgroup of G . For $\chi \in \hat{A}$, let $H_\chi = \{h \in H \mid \chi(h^{-1}ah) = \chi(a), \forall a \in A\}$. Let ρ be an irreducible representation of H_χ . Extend χ and ρ to a representation of AH_χ . Then $\text{Ind}_{AH_\chi}^G(\chi \otimes \rho)$ is an irreducible representation of G and all irreducible representations of G come from this construction.*

In our case, $G = G_N$, $H = \mathbb{Z}/2\mathbb{Z} = \langle s \rangle$, $A = \mathbb{Z}^2/N$ and $H_\chi = \{id\}$ or $\langle s \rangle$. If $H_\chi = \{id\}$, then it has only the trivial representation. In this case, $\text{Ind}_{AH_\chi}^G(\chi \otimes \rho) = \text{Ind}_A^G(\chi)$ is two dimensional such that

$$\begin{aligned} \text{Ind}_A^G(\chi)(a) &= \begin{pmatrix} 0 & \overline{\chi(\vec{v}_1)} \\ \chi(\vec{v}_1) & 0 \end{pmatrix}, \quad \text{Ind}_A^G(\chi)(b) = \begin{pmatrix} 0 & \overline{\chi(\vec{v}_1)\chi(\vec{v}_2)} \\ \chi(\vec{v}_1)\chi(\vec{v}_2) & 0 \end{pmatrix} \\ \text{Ind}_A^G(\chi)(c) &= \begin{pmatrix} 0 & \overline{\chi(\vec{v}_2)} \\ \chi(\vec{v}_2) & 0 \end{pmatrix}. \end{aligned}$$

So

$$\text{Ind}_A^G(\chi)(a) + \text{Ind}_A^G(\chi)(b) + \text{Ind}_A^G(\chi)(c) =$$

$$\begin{pmatrix} 0 & \overline{\chi(\vec{v}_1)} + \overline{\chi(\vec{v}_1)\chi(\vec{v}_2)} + \overline{\chi(\vec{v}_2)} \\ \chi(\vec{v}_1) + \chi(\vec{v}_1)\chi(\vec{v}_2) + \chi(\vec{v}_2) & 0 \end{pmatrix},$$

which has eigenvalues $\pm |\chi(\vec{v}_1) + \chi(\vec{v}_2) + \chi(\vec{v}_1)\chi(\vec{v}_2)|$.

If $H_\chi = \langle s \rangle$, then $\text{Ind}_{AH_\chi}^G(\chi \otimes \rho) = \chi\rho$. Since $\rho \in \hat{H}$ takes values in $\{1, -1\}$ and eigenvalues of the adjacency matrix are all real, we have

$$\begin{aligned} \rho\chi(a) + \rho\chi(b) + \rho\chi(c) &= \rho(s) \left(\chi(\vec{v}_1) + \chi(\vec{v}_1 + \vec{v}_2) + \chi(\vec{v}_2) \right) \\ &= |\chi(\vec{v}_1) + \chi(\vec{v}_1 + \vec{v}_2) + \chi(\vec{v}_2)| \text{ or } -|\chi(\vec{v}_1) + \chi(\vec{v}_1 + \vec{v}_2) + \chi(\vec{v}_2)|. \end{aligned}$$

We conclude that

Theorem 7. *The spectrum of X_N is $\left\{ \pm |\chi(\vec{v}_1) + \chi(\vec{v}_2) + \chi(\vec{v}_1)\chi(\vec{v}_2)| \mid \chi \in \hat{A} \right\}$.*

Recall that if the cardinality of the graph is equal to M , the HOMO eigenvalue λ_H is the $(\frac{M}{2} + 1)$ -th largest eigenvalue, the LUMO eigenvalue λ_L is the $(\frac{M}{2})$ -th largest eigenvalue and $\lambda_H - \lambda_L$ is called the HOMO-LUMO gap¹. For bipartite graphs, λ_H is equal to the smallest nonnegative eigenvalue; λ_L is equal to the largest non-positive eigenvalue and $\lambda_L = -\lambda_H$. Note that $G_N = A \amalg A$ gives a bipartite structure of X_N and so we have

Corollary 8. $\lambda_H - \lambda_L = 2 \min_{\chi \in \hat{A}} |\chi(\vec{v}_1) + \chi(\vec{v}_2) + \chi(\vec{v}_1)\chi(\vec{v}_2)|$.

A character χ of \mathbb{Z}^2 is uniquely determined by $\chi(\vec{v}_1) = \exp(i\theta_1)$ and $\chi(\vec{v}_2) = \exp(i\theta_2)$, where $\theta_1, \theta_2 \in (\mathbb{R}/2\pi\mathbb{Z})^2$. We identify $\chi \in \hat{\mathbb{Z}^2}$ with $(\theta_1, \theta_2) \in (\mathbb{R}/2\pi\mathbb{Z})^2$. The characters of \mathbb{Z}^2/N are the characters of \mathbb{Z}^2 trivial on N , so it can be identified with

$$N^\perp = \left\{ (\theta_1, \theta_2) \in (\mathbb{R}/2\pi\mathbb{Z})^2 \mid \exp(i(\theta_1 x + \theta_2 y)) = 1, \text{ for all } (x, y) \in N \right\}.$$

Consider a function f defined by

$$\begin{aligned} f(\theta_1, \theta_2) &= |\exp(i\theta_1) + \exp(i\theta_2) + \exp(i\theta_1 + i\theta_2)|^2 \\ &= 3 + 2\cos\theta_1 + 2\cos\theta_2 + 2\cos\theta_1\cos\theta_2 + 2\sin\theta_1\sin\theta_2. \end{aligned}$$

We can reformulate Corollary 8 as

Corollary 9.

$$\lambda_H - \lambda_L = \min_{(\theta_1, \theta_2) \in N^\perp} 2\sqrt{f(\theta_1, \theta_2)}.$$

This function f satisfies the following proposition used in the next section.

Proposition 10. *For $-\pi \leq \theta \leq \pi$, $f(\theta, x) \geq f(\theta, \frac{\theta}{2} + \pi)$ for all x .*

Proof. Observe that when $-\pi \leq \theta \leq \pi$, $\cos \frac{\theta}{2}$ is always nonnegative and then

$$\begin{aligned} f(\theta, x) &= 3 + 2\cos\theta + 2\cos x(1 + \cos\theta) + 2\sin\theta\sin x \\ &= 3 + 2\cos\theta + 2(1 + \cos\theta, \sin\theta) \cdot (\cos x, \sin x) \\ &= 3 + 2\cos\theta + 4\cos\frac{\theta}{2}(\cos\frac{\theta}{2}, \sin\frac{\theta}{2}) \cdot (\cos x, \sin x) \\ &\geq 3 + 2\cos\theta - 4\cos\frac{\theta}{2}, \end{aligned}$$

¹In terms of eigenvalues of the laplacian, $3 - \lambda_H$ corresponds to HOMO and $3 - \lambda_L$ corresponds to LUMO.

and the equality holds when

$$(\cos x, \sin x) = \left(-\cos \frac{\theta}{2}, -\sin \frac{\theta}{2}\right) = \left(\cos\left(\pi + \frac{\theta}{2}\right), \sin\left(\pi + \frac{\theta}{2}\right)\right).$$

□

6. FAMILIES OF TOROIDAL FULLERENES WITH GIVEN HOMO-LUMO GAP

In this section, we will show that for every natural number p not divisible by 3, there is an infinite family $\{X_{p,q}\}_q$ with the same HOMO-LUMO gap of size $\frac{2\pi}{\sqrt{3}p} + O(p^{-2})$.

Let $N_{p,q}$ be the sublattice of \mathbb{Z}^2 generated by $(p, 0)$ and $(-q, 2q)$ and $X_{p,q} = \mathcal{G}(\mathbb{Z}^2/N_{p,q} \rtimes \mathbb{Z}/2\mathbb{Z}, \{a, b, c\})$. Observe that N^\perp is generated by $\left\{\left(\frac{2\pi}{p}, \frac{\pi}{p}\right), \left(0, \frac{\pi}{q}\right)\right\}$. By Proposition 10, we have

$$\begin{aligned} \lambda_H(X_{p,q}) - \lambda_L(X_{p,q}) &= \min_{(\theta_1, \theta_2) \in N^\perp} 2\sqrt{f(\theta_1, \theta_2)} \\ &= \min_{u,v} 2\sqrt{f\left(\frac{2\pi u}{p}, \frac{\pi u}{p} + \frac{\pi v}{q}\right)} \\ &= \min_u 2\sqrt{f\left(\frac{2\pi u}{p}, \frac{\pi u}{p} + \pi\right)} \end{aligned}$$

For convenience, define $g(\theta) = f(\theta, \frac{\theta}{2} + \pi) = 3 + 2\cos\theta - 4\cos\frac{\theta}{2}$ for $-\pi \leq \theta \leq \pi$. Since $g(-\theta) = g(\theta)$, we have

$$\lambda_H(X_{p,q}) - \lambda_L(X_{p,q}) = \min_u 2\sqrt{g\left(\frac{2\pi u}{p}\right)} = \min_{0 \leq \frac{2\pi u}{p} \leq \pi} 2\sqrt{g\left(\frac{2\pi u}{p}\right)}$$

It is easy to check that $g(\theta)$ decreases in $[0, \frac{2\pi}{3}]$ and $g(\theta)$ increases in $[\frac{2\pi}{3}, \pi]$, so the minimum of $g(\frac{2\pi u}{p})$ occurs when $u = \lfloor \frac{p}{3} \rfloor$ or $\lceil \frac{p}{3} \rceil$, where $\lfloor x \rfloor$ is the floor function and $\lceil x \rceil$ is the ceiling function. On the other hand, the Taylor series expansion of $2\sqrt{g(\theta)}$ at $\theta = \frac{2\pi}{3}$ is given by

$$2\sqrt{g(\theta)} = \sqrt{3} \left| \theta - \frac{2\pi}{3} \right| + O\left(\left| \theta - \frac{2\pi}{3} \right|^2\right).$$

If $3 \nmid p$, then $\min \left\{ \left| \frac{2\pi}{p} \lfloor \frac{p}{3} \rfloor - \frac{2\pi}{3} \right|, \left| \frac{2\pi}{p} \lceil \frac{p}{3} \rceil - \frac{2\pi}{3} \right| \right\} = \frac{2\pi}{3p}$. We conclude that

Theorem 11. *If $3 \nmid p$, then $\lambda_L(X_{p,q}) - \lambda_H(X_{p,q}) = 2 \min \left\{ \sqrt{g\left(\frac{2\pi}{p} \lfloor \frac{p}{3} \rfloor\right)}, \sqrt{g\left(\frac{2\pi}{p} \lceil \frac{p}{3} \rceil\right)} \right\} = \frac{2\pi}{\sqrt{3}p} + O(p^{-2})$, which is independent of q .*

7. IMBEDDING GRAPH INTO THREE DIMENSIONAL SPACE

For the purpose of real world applications, it is important to design fullerenes which have a good imbedding in three dimensional space with small potential energy. The first constraint of such imbedding is that the length of each edge should be almost equal. This constraint will be satisfied if the imbedding of fullerene graphs is isometric. Note that for the lattices $N'_{p,q} = N_{p,q}(\vec{e}_0)$ on the Euclidean plane \mathbb{R}^2 has a fundamental domain Σ spanned by the orthogonal basis $p\vec{v}_1$ and $-q\vec{v}_1 + 2q\vec{v}_2$. Choose the length of \vec{v}_1 as the unit of length. The

width of Σ equals p ; its length equals $2\sqrt{3}q$. The fullerene graphs $X_{p,q}$ is obtained from the hexagon tiling Y in \mathbb{R}^2 quotient by the lattices $N'_{p,q}$, so it suffices to find a map from $\mathbb{R}^2/N'_{p,q}$ to three dimensional space, which induces an imbedding of $X_{p,q}$ to three dimensional space. Consider the standard map $F(u, v) = (x(u, v), y(u, v), z(u, v))$ from Σ to a torus, where

$$\begin{cases} x(u, v) &= \left(R + r \cos\left(\frac{2\pi u}{p}\right)\right) \cos\left(\frac{\pi v}{\sqrt{3}q}\right), \\ y(u, v) &= \left(R + r \cos\left(\frac{2\pi u}{p}\right)\right) \sin\left(\frac{\pi v}{\sqrt{3}q}\right), \\ z(u, v) &= r \sin\left(\frac{2\pi u}{p}\right), \end{cases}$$

and R and r are some constants. In order that F is an isometry, it should satisfy $\langle F_u, F_v \rangle = 0$, $\langle F_u, F_u \rangle = \frac{4\pi^2 r^2}{p^2} = 1$ and $\langle F_v, F_v \rangle = \frac{\pi^2 R^2}{3q^2} \left|1 + \frac{r}{R} \cos\left(\frac{2\pi u}{p}\right)\right|^2 = 1$, which is impossible. However, we can simply let $r = \frac{p}{2\pi}$ and $R = \frac{\sqrt{3}q}{\pi}$, such that $\langle F_u, F_u \rangle = 1$ and $\langle F_v, F_v \rangle = \left|1 + \frac{p}{2\sqrt{3}q} \cos\left(\frac{2\pi u}{p}\right)\right|^2$. Then F is close to an isometry when $\frac{p}{q}$ is small. Thus with p fixed and q increasing, we can increase the stability of the molecule without changing the HOMO-LUMO gap. Note that when $\frac{p}{q} \rightarrow 0$, the toroidal fullerene becomes a carbon nanotube.

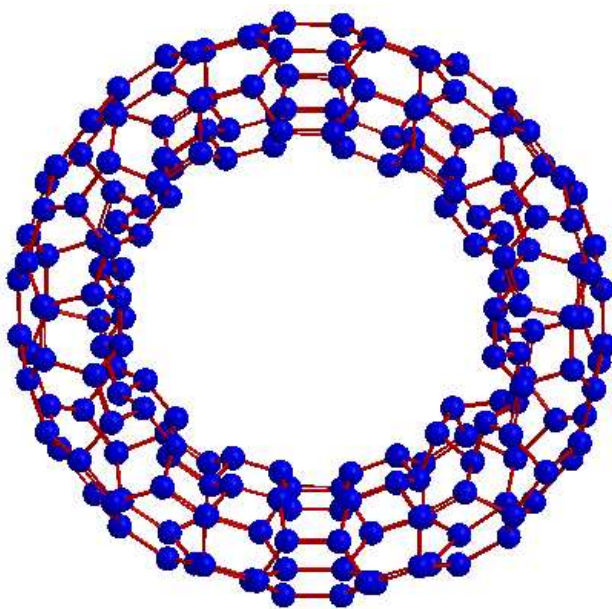


Figure 8: $p = 5, q = 10$

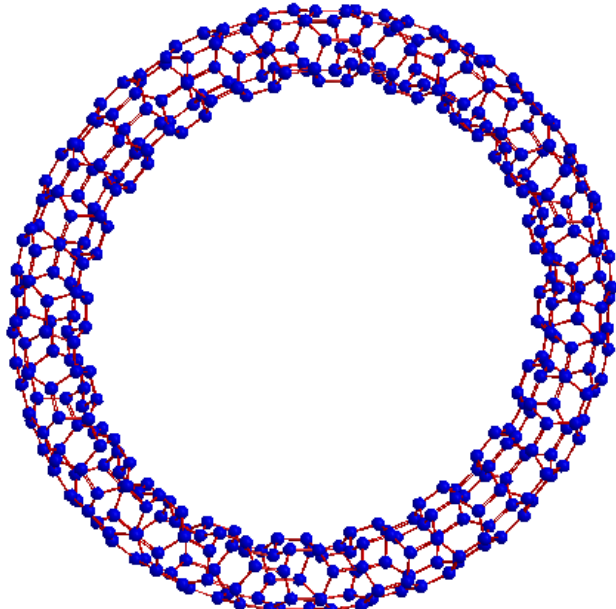


Figure 9: $p = 5, q = 20$

8. ACKNOWLEDGEMENT

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REFERENCES

- [1] W. B. Smith, *Introduction to Theoretical Organic Chemistry and Molecular Modelling*, Wiley-VCH, 1996
- [2] W. Fowler, P. Hansen, G. Caporossi and A. Soncini, *Polyynes with maximal HOMO-LUMO gap*, Chemical Physical Letters **342** (2001), 105-112.
- [3] W. Fowler and I. Steer, *The Leapfrog Principle: A Rule for electron Counts of Carbon Clusters*, J. Chem. Soc., Chem. Commun. (1987), 1403-1405.

- [5] E. Manolopoulos, R. Woodall and W. Fowler, *Electronic Stability of Fullerenes: Eigenvalue Theorems for Leapfrog Carbon Clusters*, J. Chem. Soc. Faraday Trans. **88**(17) (1992), 2427-2435.
- [4] F. Zhang and C. An, *Acyclic molecules with greatest HOMO-LUMO separation* Discrete Applied Mathematics, **98**(1999) 165-171.
- [6] J. E. Avron and J. Berger. *Tiling rules for toroidal molecules*, Phys. Rev. A, 51(2):1146-1149, Feb 1995.
- [7] J. Berger and J. E. Avron, *Classification scheme for toroidal molecules*, J. Chem. Soc. Faraday Trans., **91**(22):4037-4045, 1995.
- [8] R. Tamura, M. Ikuta, T. Hirahara, and M. Tsukada. *Positive magnetic susceptibility in polygonal nanotube tori*, Phys. Rev. B, 71(4):045418, Jan 2005.
- [9] J. Serre, *Linear representations of finite groups*, Springer-Verlag (1997).

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